IN THE CLAIMS:

1.   (Presently amended) A method for calculating a global hydrophobic moment of a tertiary protein structure comprising a plurality of residues, the method comprising the steps of:

5   calculating a centroid of residue centroids;

               using the centroid of residue centroids as a spatial origin of a global linear hydrophobic moment;

               calculating a first-order hydrophobic moment;

               enhancing correlation between residue centroid magnitude and residue
10   solvent accessibility, wherein the correlation between residue centroid magnitude and residue solvent accessibility is enhanced using a distance metric;

               using the first-order hydrophobic moment and the enhanced correlation between residue centroid magnitude and residue solvent accessibility to define the global linear hydrophobic moment, wherein each of the residue centroids contributes a
15   magnitude and direction to the global linear hydrophobic moment;

               using the global linear hydrophobic moment to characterize an amphiphilicity of a tertiary protein structure; and

               outputting the global linear hydrophobic moment to ~~at least one of~~ a user~~, a display and one or more additional computers on a network~~.

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2.   (Canceled)

3.   (Original) The method of claim 1, wherein the correlation between residue centroid magnitude and residue solvent accessibility is enhanced using an ellipsoidal
25   metric.

4.   (Original) The method of claim 1, wherein the correlation between residue centroid magnitude and residue solvent accessibility is enhanced using a solvent accessibility metric.

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5. (Original) The method of claim 1, wherein the centroid of residue centroids represents a geometric center of the tertiary protein structure.

6. (Cancelled)

7. (Original) The method of claim 1, wherein the global linear hydrophobic moment characterizes a magnitude of amphiphilicity of the tertiary protein structure.

8. (Original) The method of claim 1, wherein the global linear hydrophobic moment characterizes a direction of amphiphilicity of the tertiary protein structure.

9. (Original) The method of claim 1, wherein the global linear hydrophobic moment is used to identify functional regions of the tertiary protein structure.

10. (Cancelled)

11. (Cancelled)

12. (Cancelled)

13. (Cancelled)

14. (Presently amended) An apparatus for calculating a global hydrophobic moment of a tertiary protein structure comprising a plurality of residues, the apparatus comprising:

    a memory; and

    at least one processor operative to:

    calculate a centroid of residue centroids;

    use the centroid of residue centroids as a spatial origin of a global linear hydrophobic moment;

    calculate a first-order hydrophobic moment;

enhance correlation between residue centroid magnitude and residue solvent accessibility, wherein the correlation between residue centroid magnitude and residue solvent accessibility is enhanced using a distance metric;

use the first-order hydrophobic moment and the enhanced correlation between residue centroid magnitude and residue solvent accessibility to define the global linear hydrophobic moment, wherein each of the residue centroids contributes a magnitude and direction to the global linear hydrophobic moment;

use the global linear hydrophobic moment to characterize an amphiphilicity of a tertiary protein structure; and

output the global linear hydrophobic moment to ~~at least one of~~ a user, ~~a display and one or more additional computers on a network~~.

15. (Original) The apparatus of claim 14, wherein the centroid of the residue centroids represents a geometric center of the tertiary protein structure.

16. (Cancelled)

17. (Original) The apparatus of claim 14, wherein the global linear hydrophobic moment is used to identify functional regions of the tertiary protein structure.

18. (Canceled)

19. (Original) The apparatus of claim 14, wherein the correlation between residue centroid magnitude and residue solvent accessibility is enhanced using an ellipsoidal metric.

20. (Original) The apparatus of claim 14, wherein the correlation between residue centroid magnitude and residue solvent accessibility is enhanced using a solvent accessibility metric.

21. (Presently amended) An article of manufacture for calculating a global hydrophobic moment of a tertiary protein structure comprising a plurality of residues, comprising:

a computer-readable medium having computer-readable code embodied thereon, the computer-readable code comprising:

a step to calculate a centroid of residue centroids;

a step to use the centroid of residue centroids as a spatial origin of a global linear hydrophobic moment;

a step to calculate a first-order hydrophobic moment;

a step to enhance correlation between residue centroid magnitude and residue solvent accessibility, wherein the correlation between residue centroid magnitude and residue solvent accessibility is enhanced using a distance metric;

a step to use the first-order hydrophobic moment and the enhanced correlation between residue centroid magnitude and residue solvent accessibility to define the global linear hydrophobic moment, wherein each of the residue centroids contributes a magnitude and direction to the global linear hydrophobic moment;

a step to use the global linear hydrophobic moment to characterize an amphiphilicity of a tertiary protein structure; and

a step to output the global linear hydrophobic moment to ~~at least one of~~ a user~~, a display and one or more additional computers on a network~~.